AEC-NASA TECH BRIEF

Computer Program Calculates the Effective Temperature for a Crystalline Solid (DETS)

The problem:

When a gas model is used to calculate a thermal neutron scattering kernel for reactor design calculations, the temperature is the only free parameter. The evaluation of this effective temperature involves use of the Debye temperature. It is not usually known, however, whether the Debye temperature from the specific heat or that from the Debye-Waller factor should be used if the two differ.

The solution:

A computer program which computes and prints out both the Debye and resulting effective temperatures for each Debye model-dependent average energy per vibrational mode, Debye-Waller factor, and specific heat.

How it's done:

The program calculates by the trapezoidal rule the normalized values of the frequency distribution. From these values, the trapezoidal rule is used by separate subroutines to calculate the frequency distribution-based integrals for average energy per vibrational mode, EBAR, the Debye-Waller factor, DBWF, and the specific heat, CV.

Each of these values is then used by a separate subroutine in iteration on the upper limits of a new integral for each, EBAR, DBWF and CV. The new integrals all depend on the Debye model. The upper limits are changed to force the Debye model-dependent values sufficiently close to the frequency distribution-dependent values. The Debye temperature is then calculated from each Debye model-dependent EBAR, DBWF and CV, combined with its corresponding altered upper limit.

The integral for effective temperature can then be solved by Simpson's Rule using the Debye temperature from either CV or DBWF or both.

Detailed printout includes EBAR, DBWF and CV, from both the frequency distribution and Debye model-dependent cases, along with subsequent effective temperatures and all Debye temperatures.

Notes:

1. This program is written in Fortran IV for use on the CDC-6600 computer.
2. Inquiries concerning this program may be made to:
   COSMIC
   Computer Center
   University of Georgia
   Athens, Georgia 30601
   Reference: B69-10036

Patent status:

No patent action is contemplated by AEC or NASA.

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